

α (low) Quartz (SiO_2) Structure: A2B_hP9_152_c_a-001

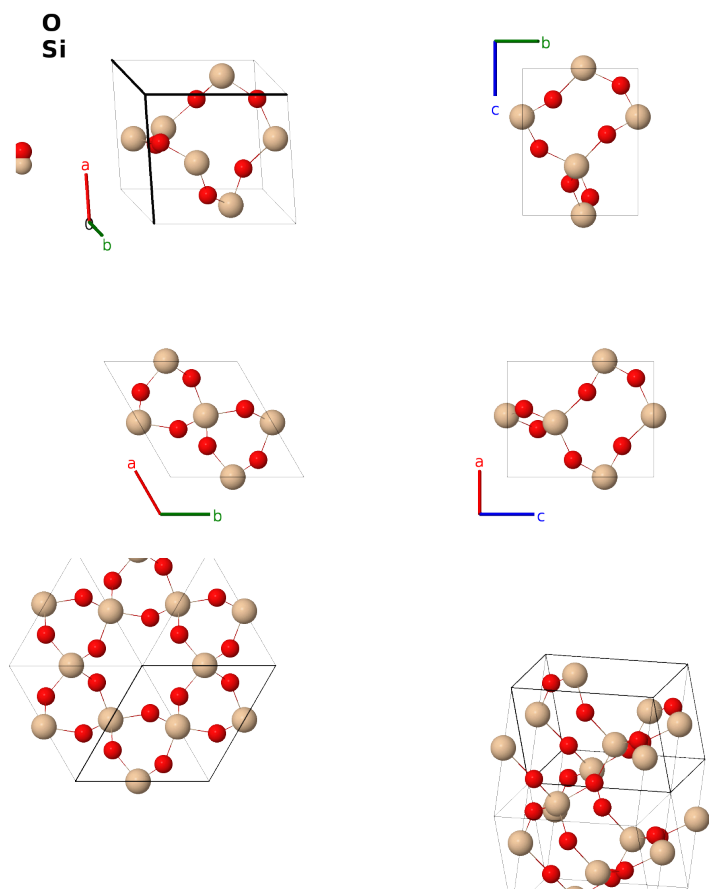
This structure previously used the label(s) **A2B_hP9_152_c_a**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/P53L>

https://aflow.org/prototype-encyclopedia/A2B_hP9_152_c_a-001



Prototype	O_2Si
AFLOW prototype label	A2B_hP9_152_c_a-001
Mineral name	quartz
ICSD	67121
CCDC	1629160
Pearson symbol	hP9
Space group number	152

Space group symbol $P3_121$

AFLOW prototype command `aflow --proto=A2B_hP9_152_c_a-001`
`--params=a, c/a, x1, x2, y2, z2`

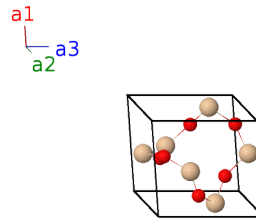
Other compounds with this structure

GeO₂

- When $x_1 = 1/2$, $y_2 = 2x_2$, and $z_2 = 1/2$ this transforms into the high β -quartz ($C8$) structure, with the phase transformation occurring at 573°C (Wright, 1981).
- This structure can also be found in the enantiomorphic space group $P3_221$ #154.
- More information about SiO₂ structures can be found in our article on SiO₂ and AlPO₄.

Trigonal (Hexagonal) primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_3$	$=$	$\frac{1}{2}ax_1 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_1 \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}$	(3a)	Si I
$\mathbf{B}_2$	$= x_1 \mathbf{a}_2 + \frac{2}{3} \mathbf{a}_3$	$=$	$\frac{1}{2}ax_1 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_1 \hat{\mathbf{y}} + \frac{2}{3}c \hat{\mathbf{z}}$	(3a)	Si I
$\mathbf{B}_3$	$= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2$	$=$	$-ax_1 \hat{\mathbf{x}}$	(3a)	Si I
$\mathbf{B}_4$	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_2 + y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_2 - y_2) \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B}_5$	$= -y_2 \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 + (z_2 + \frac{1}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_2 - 2y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{3}) \hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B}_6$	$= -(x_2 - y_2) \mathbf{a}_1 - x_2 \mathbf{a}_2 + (z_2 + \frac{2}{3}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_2 - y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_2 \hat{\mathbf{y}} + \frac{1}{3}c(3z_2 + 2) \hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B}_7$	$= y_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_2 + y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_2 - y_2) \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B}_8$	$= (x_2 - y_2) \mathbf{a}_1 - y_2 \mathbf{a}_2 - (z_2 - \frac{2}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_2 - 2y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} - \frac{1}{3}c(3z_2 - 2) \hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B}_9$	$= -x_2 \mathbf{a}_1 - (x_2 - y_2) \mathbf{a}_2 - (z_2 - \frac{1}{3}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_2 - y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_2 \hat{\mathbf{y}} - c(z_2 - \frac{1}{3}) \hat{\mathbf{z}}$	(6c)	O I

References

- [1] R. M. Hazen, L. W. Finger, R. J. Hemley, and H. K. Mao, *High-pressure crystal chemistry and amorphization of α -quartz*, Solid State Commun. **72**, 507–511 (1989), doi:10.1016/0038-1098(89)90607-8.
- [2] A. F. Wright and M. S. Lehmann, *The Structure of Quartz at 25 and 590°C Determined by Neutron Diffraction*, J. Solid State Chem. **36**, 371–380 (1981), doi:10.1016/0022-4596(81)90449-7.

Found in

[1] J. Donohue, *The Structures of the Elements* (Robert E. Krieger Publishing Company, New York, 1974).

First cited in

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